Software Status Bulletin
G3336AA Qualitative Analysis Software rev. B.06.00 SP1

Revision Log:

Revision Date	Reason For Update
4/5/2013	**Initial revision**

1. Overview

The purpose of this document is to list known problems in the software and any known workarounds or recovery paths.

2. Known Problem Summary

The following is a summary of the known problems in the software. This is not an exhaustive list, but is a list of the problems a customer is most likely to encounter. This list cross-references items in our Defect tracking database.

Issue #	Title
172494	Manual integration of UV chromatogram with General Integrator results in strange baselines
180034	Localization: In the Japanese version, "Hide any Current Empty Columns" does not work in the Compound List
186897	Hitting F1 in the "Enter Filter Criteria" dialog box does not display the proper help page
188285	Diff(ppm) and Diff(mDA) show incorrect values in the MS peaklist when formula generation results are cleared
189804	In Accurate Mass library search, entering a ".L" or ".XML" file path in the textbox and trying to perform a search will throw an exception
190451	Trying to load a data file in Qual while acquiring will flag an error
190959	For targeted MSMS and FBF, repeated calls for extracting complete result set adds an MSMS spectrum
191172	Localization: Online Help - The Japanese online help for Report Designer is not translated properly
192489	Fragment formula annotation should show MFG results if best hit is neither Library ID hit nor Manual ID hit for user spectra
192551	"Restore to last saved values" from file does not work for Peak absolute height
192559	Methods fail to load after changing a "Message Box Options" dialog setting
192601	Tab selection in the Maximum Entropy tab of Method Editor -> Find by Protein Deconvolution is out of order
192609	TAB order navigation between fields is irregular in Find by Formula Options -> Result Filters
192615	"Copy deconvolution settings to method" is allowed for Resolved Isotope Deconvolution but will crash Qual
192958	Protein Digest matching rules field becomes blank and rules become unavailable for selection upon certain actions
193050	Selecting multiple compounds in the Data Navigator pane will not include the first compound selected

193063	Changing the "Source of formulas to confirm" in the Formula Source tab of FbF - Options also adds a blue triangle to the "Find by Formula - Chromatograms" section in Method Explorer
193065	"Create Compound from Highlighted Range on Deconvoluted Spectrum" is not supported for Isotope Resolved Deconvoluted spectra and will cause crashes
193067	The LMFE tab is not greyed out when "small molecule" is selected for "Target data type" in the method editor
193228	Once the Compare Protein Digest Files wizard process starts it cannot be canceled.
193229	Message needs to be displayed before the process completes
193338	"Protease digest location" indicators are removed after canceling the Edit Digest Reagents dialog
193339	Digest List: Define and Match Sequence pane loses data
193378	An error message found in: Method Editor > Find Compound by Formula - Options > Positive Ions tab, is not translated into Chinese
193470	Changing back to the default printer does not work for deconvolution results
193486	Occasional exception flags when changing workflows using data files not in the customer's Home path
193489	Compound list table print-out is illegible for some settings
193630	Function: changed value messages are missing in Method Editor > Find Compound by Formula - Options > Results tab
193718	No blue triangles are added to the method editor for search accurate mass library when switching search accurate mass library to search unit mass library
193755	Find by Integration -> Adjust Delay Time tab contains misaligned fields
194031	Localization Issue: Error message contains both English and Japanese strings
194053	Displaying overlaid MRMs then switching from minutes to scans may cause an error
194449	All Ions MS/MS (AIM) - Visualization in the Compound Fragment Spectrum Results window in Compound Details View (CDV) is incorrect
194537	Cell borders are missing in BioConfirm Protein Compound reports
194539	Oligonucleotide reports will contain some cosmetic discrepancies
194702	Localization: "Acquisition Time" axis label in the Chromatogram Result plot is not translated into Japanese
194817	Scrolling anomaly exists in Digest Comparative Analysis window
194818	Multiple rows cannot be highlighted in Compound Compare List table
194819	Chromatogram selection in Digest Compare Results does not work correctly
194820	Chromatogram Compare report generation does not work properly
194821	Mass Spectrum Compare Results printing has several issues
194822	MSMS Spectrum Compare Results pane has multiple print issues
195162	F1 doesn't show help in Isotope Distribution Calculator
195492	In CDV with BioConfirm ProteinDigest results - scrolling to the end of the Compound List then back up to last seq. match will cause the cursor to slowly self scroll back to end of list/last compound
195643	Layouts in Compound Details View (CDV) and Navigator View (NV) do not save and preserve which PANE is on top if multiple windows are TABBED.
195649	Changing workflows does not work if "Save current method" is checked in the dialog box
195773	EIC Peak List table does not get updated in tandem with compound selection
195933	If only "Other (CE)" is marked in the User Interface Configuration dialog box, menu items and method editor sections are not chosen consistently
196295	Exception occurs in METLIN - Navigator View while repeatedly printing reports over and over for thousands of compounds per data file

196296	Exception on generating Compound Report for ForensicsTox Find by Formula analysis
196507	Color coding of ions based on Fragment Annotation is still displayed when Fragment Annotation is unchecked.
196599	All Ions: ?? appearing on "delete" and "extract complete result set"
196720	MS/MS Formula details disappear when selecting a different "Best" Formula after running Find Compounds by Auto MS/MS and MFG
196721	The "Hide Empty Columns" tool button in the Compound List works for the first level, but not the second level.
196722	Compound List column order for BioConfirm Protein Digest is randomly ordered
196831	In Compound Details View, right-clicking near an axis in the Compound Chromatogram window will throw an error
196842	Merged Spectrum ID Results with LibSearch-MFG results - only the highest Lib Score hit has MFG results and Isotope pattern although all are labeled as merged LibSearch-MFG
196930	Spectrum not seen on printed report when grid lines are turned on.
196936	A Compound report after running MFE + MFG contains 3 columns with the identical formula
196939	When run as a Compound Automation Step, Find Compounds by MRM produces a TIC Scan with NO DATA POINTS
197052	Qual crashes when Find by Protein Deconvolution is attempted under specific conditions
197054	Protein compound report with two data sets may fail
197064	Compound Details View (CDV) - Exception when trying to access the Add/Remove Columns dialog in the 4th level of the Compound ID Results Window
197212	Tooltip of Method Explorer is not properly updated
197263	Annotation does not work properly for a HighE spectrum
197273	Formula and Mass Calculators do not contain GC/Q-TOF parameters when a GC/Q-TOF method is loaded
197404	Chemical Data Dictionary Editor tabs do not display the relevant help topics
197514	Wizard pages do not display relevant help topics

3. Known Problems Detailed Description

The following is the detailed descriptions of the known problems in the Qualitative Analysis software. This section includes more extensive information from our defect tracking database. This section also includes any known workarounds or recovery paths

Issue # 172494	
Title	Manual integration of UV chromatogram with General Integrator results in strange baselines
Description	When the user manually integrates a UV chromatogram with the General integrator, it creates very strange baselines. The problem only appears to happen on peaks with an RT > 6 minutes. If you manually integrate the peaks before 6 minutes, it works fine.

Issue # 180034

Title	Localization: In the Japanese version, "Hide any Current Empty Columns" does not work in the Compound List
Description	1. Load sulfa-posESIautoMSMS-c.d 2. Method Editor > Find Compound by Formula > Formula Source tab 3. Select Database & mass(e) 4. Run Find Compounds by Formula 5. Show Compound list and Compound Identification Result 6. Select "Hide any current Empty Column" to hide empty columns. Does not work in Compound List view or Compound Identification Results views. Note: This applies to the Japanese version.

Issue # 186897	
Title	Hitting F1 in the "Enter Filter Criteria" dialog box does not display the proper help page
Description	Pressing F1 in the "Enter Filter Criteria" dialog box will display the main help page instead of the proper topic's page.

Issue # 188285	
Title	Diff(ppm) and Diff(mDA) show incorrect values in the MS peaklist when formula generation results are cleared.
Description	Generate formula for a spectrum. Some rows with Diff(ppm) and Diff(mDA) in the MS peak list table there will contain gibberish. Clearing the spectrum identification results will then result in the MS peak list table containing many rows of "Diff(ppm)" and "Diff(mDA)" filled with gibberish.

Issue # 189804	
Title	In Accurate Mass library search, entering a ".L" or ".XML" file path in the textbox and trying to perform a search will throw an exception
Description	1. Open a datafile (eg: _2_1CP_2^2_25_F.D) 2. Perform "Find Compounds by Chromatogram Deconvolution" 3. Select the compounds and go to Method Explorer -> Identify Compounds -> Search Accurate Mass Library 4. Enter a .L library path (eg: C:\DATABASE\NIST08.L) in the textbox manually (without browsing) and click "Search Library for Compounds". The following exception is thrown: "Program: Agilent MassHunter Workstation Software Qualitative Analysis B.06.00 Build Configuration: Release Message: Object reference not set to an instance of an object. Stack Trace: Server stack trace: at Agilent.MassSpectrometry.DataAnalysis.UnitMassSearch.DoSearch(ICompound iCpd, IMassSpectrum iMsSpec, IUnitsConverter iUnitsConverter, Double appDelayTime,

	ILibrarySearchSettings libSearchSettings) in z:\Archer\core\CoreSpectralLibrarySearch\SpectralLibrarySearch\Algorithms\UnitMassSearch.cs:line 59 at Agilent.MassSpectrometry.DataAnalysis.SpectralLibrarySearch.Agilent.MassSpectrometry.DataAnalysis.ISpectralLibrarySearch.Search(ICompound compound, ISpectrum spectrum, ILibrarySearchSettings searchSettings) in z:\Archer\core\CoreSpectralLibrarySearch\SpectralLibrarySearch\Algorithms\SpectralLibrarySearch.cs:line 307 at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualCommandBase.LibSearchForCompoundSpec(ISpectralLibrarySearch libSearch, ILibrarySearchSettings searchSettings, DataItem cpdDataItem, DataItem[] specDataItem) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualCommandBase.DoCpdLibrarySearch(DataItem[] selectedItems, LimitProgressTracker overallProgress) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CmdLibaraySearchCompound.DoSpecialized() at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CmdApply.DoSpecialized() at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualCommandBase.Do() at Agilent.MassSpectrometry.CommandModel.CommandHistory.Invoke(ICommand cmd) in z:\Archer\core\Command\commandmodel\commandhistory.cs:line 337 at System.Runtime.Remoting.Messaging.StackBuilderSink._PrivateProcessMessage(IntPtr md, Object[] args, Object server, Int32 methodPtr, Boolean fExecuteInContext, Object[]& outArgs) at System.Runtime.Remoting.Messaging.StackBuilderSink.PrivateProcessMessage(RuntimeMethodHandle md, Object[] args, Object server, Int32 methodPtr, Boolean fExecuteInContext, Object[]& outArgs) at System.Runtime.Remoting.Messaging.StackBuilderSink.AsyncProcessMessage(IMessage msg, IMessageSink replySink) Exception rethrown at [0]: at System.Runtime.Remoting.Proxies.RealProxy.EndInvokeHelper(Message reqMsg, Boolean bProxyCase) at System.Runtime.Remoting.Proxies.RemotingProxy.Invoke(Object NotUsed, MessageData& msgData) at Agilent.MassSpectrometry.CommandModel.CommandHistory.InvokeCommand.EndInvoke(IAsyncResult result) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.AppManager.EndInvoke(IAsyncResult result) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualForm.OnAsyncCallBack(IAsyncResult asyncResult) in z:\Archer\qual\presentation\AgtQual\QualFormP1.cs:line 2369"

Issue # 190451	
Title	Trying to load a data file in Qual while acquiring will flag an error
Description	If a dMRM or tMRM data file is loaded into qual while it is simultaneously being acquired, an exception will be thrown

Issue # 190959	
Title	For targeted MSMS and FBF, repeated calls for extracting complete result set adds an MSMS spectrum
Description	1) Open sulfas_PosTargetedMSMS.d 2) Load default.m. 3) Run find compounds by targeted MSMS. 4) Each compound will have a TIC and Product ion scan extracted. 5) Run extract complete result set: a MS scan and Product ion scan is added. 6) Run extract complete result set again: another Product ion scan (same as previous) is added. This also happens with FbF.

Issue # 191172	
Title	Localization: Online help file Index is all gibberish and cannot be searched in Japanese
Description	Online help Index tab is all gibberish. Additionally, cannot search in Japanese with search tab.

Issue # 192489	
Title	Fragment formula annotation should show MFG results if best hit is neither Library ID hit nor Manual ID hit for user spectra
Description	1) For a user spectra that has a library (and/or manual id) id, MFG, or database search results. 2) Check fragment formula annotation. 3) If the "best" hit is among library id or manual id then FFA (fragment formula annotation) should be executed and the spectra should be colored accordingly 4) However, if the user selects MFG or Dbase ID as "best" hit then peaks that should be labelled with MFG results are not labeled properly (if it is calculated for that spectra). -Additionally, any Red or Green labeled peaks do not revert to a single color.

Issue # 192551	
Title	"Restore to last saved values" from file does not work for Peak absolute height
Description	1) Load default.m or any other method 2) Open: Method Editor - Deconvolute (MS): Protein. 3) In the Maximum Entropy tab select "Peak absolute height." 4) Click on the "Restore to last saved values from file" icon in the method editor toolbar. The radio button will not change back to the "Peak signal-to-noise" parameter.

Issue # 192559	
Title	Methods fail to load after changing a "Message Box Options" dialog setting
Description	1) Close any exisiting data file. 2) Ensure Method check box is not marked in Configuration -> Message Box Options. 3) Open the previously closed data file with "Load results method" selected.

	4) In the Save dialog (for method changes) that is displayed select both check boxes: "Save as needed" and "Do not show this box again" 5) Click No. 6) Click on the "Open Method" icon in the Find by Protein Method Editor. 7) In the Open Method dialog box, select a user created method and click Open. 8) In the Save Method dialog box, rename the file and save the method. The new method name will be displayed in the title bar. 9) Click on the Open Method icon in the Find by Protein method editor. 10) Select another method and click Open. The selected method will not load. Subsequent attempts will also fail and Qual will have to be forced out via the Task Manager.

Issue # 192601	
Title	Tab selection in the Maximum Entropy tab of Method Editor -> Find by Protein Deconvolution is out of order
Description	1) Method Editor -> Find by Protein Deconvolution and proceed to the Maximum Entropy tab. 2) Whilst using the tab key to change fields, after "Limit to the largest parameter", the tab selection leaves the Method Editor before continuing with the rest of the fields.

Issue # 192609	
Title	TAB order navigation between fields is irregular in Find by Formula Options -> Result Filters
Description	For any TOF datafile: the TAB order navigation between fields is irregular in Find by Formula Options -> Result Filters -If the user enters a new valid value for Warn if score is < _____, hittnig the TAB key highlights the text description for the checkbox at the bottom of the pane "Do not match if the (unobserved" second ions abundance is expected to be > _____." instead of the actual field. -Hitting the TAB key highlights the text for the first checkbox in the pane "Only generate Compounds to matched formulas" and not the actual field.

Issue # 192615	
Title	"Copy deconvolution settings to method" is allowed for Resolved Isotope Deconvolution but will crash Qual
Description	"Copy deconvolution settings to method" is intended for Peak Modeling Deconvolution and Max Entropy Deconvolution. Trying to use this on Resolved Isotope Deconvolution will crash Qual.

Issue # 192958	
Title	Protein Digest matching rules field becomes blank and rules become unavailable for selection upon certain actions

Description	1) Load enolase digest data (or any other digest data file). 2) Open Sequence -> Edit matching rules. 3) Use the Ctrl key deselect all the matching rules and click OK or Cancel. When the dialog is re-opened, all the rules are removed and are also not available for selection. This happens with Protein matching rules as well.

Issue # 193050	
Title	Selecting multiple compounds in the Data Navigator pane will not include the first compound selected.
Description	1) In Navigator View, highlight the first compound. 2) Hold shift key and clicke the fourth compound in the list in the Data Navigator window. 3) Instead of compounds 1 – 4 being highlighted, only compounds 2 – 4 are highlighted. If compounds 2-4 are selected, only compounds 3 and 4 are highlighted.

Issue # 193063	
Title	Changing the "Source of formulas to confirm" in the Formula Source tab of FbF - Options also adds a blue triangle to the "Find by Formula - Chromatograms" section in Method Explorer
Description	Changing the "Source of Formulas to Confirm" in the Formula Source tab of FbF - Options will also add a blue triangle to the "FbF - Chromatograms" section in the Method Explorer pane. This does not impact usability.

Issue # 193065	
Title	"Create Compound from Highlighted Range on Deconvoluted Spectrum" is not supported for Isotope Resolved Deconvoluted spectra and will cause crashes
Description	-Find > Create Compound from Highlighted Range on Deconvoluted Spectrum > Add Highest Peak will throw: “Qualitative Analysis encountered an error” message. **Temporary Solution:** This is not a supported feature for RID. **Fix Information:** This option for RID will be disabled in future.

Issue # 193067	
Title	The LMFE tab is not greyed out when "small molecule" is selected for "Target data type" in the method editor
Description	LMFE tab is still editable when small molecule items are selected for "Target data type" in the method editor.

Issue # 193228	
Title	Once the Compare Protein DigestFiles wizard process starts it cannot be canceled.
Description	1) Open enolase digest chip data files. 2) Open: Compare Protein Digest Files -> Find Results, Identify and Compare. 3) Load the data files in the first page of the wizard and click Finish. After it starts, click on the Cancel button in the progress dialog. The run does not end and the user has to wait for it to complete. Can take up to 30 mins or longer with more than 2 data files.

Issue # 193229	
Title	Message needs to be displayed before the process completes
Description	1) Open enolase digest chip data files. 2) Open: Compare Protein Digest Files -> Find Results, Identify and Compare. 3) Load the data files in the first page of the wizard. 4) Ensure that there is no sequence file or mass list in the Define and Match Sequence page of wizard. 5) Click Finish. The message "Match Operation was not started. Please enter a sequence in the Match Sequences..." appears at the end of the process, instead right after the Finish button is clicked.

Issue # 193338	
Title	"Protease digest location" indicators are removed after canceling the Edit Digest Reagents dialog
Description	1) Import any digest sequence file into the Sequence editor. 2) Using the right-click context menu, open “Edit Digest Reagents”. Click OK. 3) The digest markings are placed in the sequence. 4) Re-open the dialog and add another reagent from “Available” to “Select” field. Click Cancel. All the previous digest markings are removed.

Issue # 193339	
Title	Digest List: Define and Match Sequence pane loses data
Description	Digest List: Define and Match Sequence pane loses data after Clicking OK in the Edit Digest Reagents dialog. After that it does not get updated if a change is made to the sequence. The same thing occurs in the Edit Modifications dialog.

Issue # 193378

Title	An error message found in: Method Editor > Find Compound by Formula - Options > Positive Ions tab, is not translated into Chinese
Description	The error message in the mentioned tab states: "Ranges must be ordered (minimum - maximum)." It is not translated into Chinese like the rest of the dialog box.

Issue # 193470	
Title	Changing back to the default printer does not work for deconvolution results
Description	1) Configure the computer with at least two printers. 2) Load a data file with deconvolution results. 3) Right click in the results pane and select Print. Printing with the default printer properly sends to the default printer. 4) Change the printer name field to a second printer in the Print dialog and click OK. This properly sends to the second printer. 5) Reopen the print dialog and change the Printer name field back to default and click OK. This will not properly send to the default printer. Instead, the second printer is still used.

Issue # 193486	
Title	Occasional exception flags when changing workflows using data files not in the customer's Home path
Description	1) Configure User Interface for GC-QTOF 2) Load TOF type file such as MSD_mix_4stds_DG_spl200_03.D 3) Use General or GC-QTOF workflow 4) Run Find by Integration 5) Run a library search with: "demo.L" 6) Save results 7) Configure General Workflow. - Clicking OK MAY then cause Qual to crash with the following exception: Date and Time: 8/28/2012 9:55 AM Program: Agilent MassHunter Workstation Software Qualitative Analysis B.06.00 Build Configuration: Release Message: Error creating window handle. Stack Trace: at System.Windows.Forms.NativeWindow.CreateHandle(CreateParams cp) at System.Windows.Forms.Control.CreateHandle() at System.Windows.Forms.Control.CreateControl(Boolean fIgnoreVisible) at System.Windows.Forms.Control.CreateControl() at System.Windows.Forms.Control.OnVisibleChanged(EventArgs e) at System.Windows.Forms.Control.OnVisibleChanged(EventArgs e) at System.Windows.Forms.Form.OnVisibleChanged(EventArgs e) at System.Windows.Forms.Control.SetVisibleCore(Boolean value) at System.Windows.Forms.Form.SetVisibleCore(Boolean value) at System.Windows.Forms.Application.ThreadContext.RunMessageLoopInner(Int32 reason, ApplicationContext context) at System.Windows.Forms.Application.ThreadContext.RunMessageLoop(Int32 reason,

	ApplicationContext context) at System.Windows.Forms.Form.ShowDialog(IWin32Window owner) at Agilent.MassSpectrometry.DataAnalysis.BaseErrorDialog.ShowException(Exception exception) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualForm.OnQualFormThreadExceptionEvent(Object sender, ThreadExceptionEventArgs e) at System.Windows.Forms.Application.ThreadContext.OnThreadException(Exception t) at System.Windows.Forms.NativeWindow.Callback(IntPtr hWnd, Int32 msg, IntPtr wparam, IntPtr lparam) at System.Windows.Forms.UnsafeNativeMethods.DispatchMessageW(MSG& msg) at System.Windows.Forms.Application.ComponentManager.System.Windows.Forms.UnsafeNativeMethods.IMsoComponentManager.FPushMessageLoop(IntPtr dwComponentID, Int32 reason, Int32 pvLoopData) at System.Windows.Forms.Application.ThreadContext.RunMessageLoopInner(Int32 reason, ApplicationContext context) at System.Windows.Forms.Application.ThreadContext.RunMessageLoop(Int32 reason, ApplicationContext context) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.Program.Main(String[] args)

Issue # 193489	
Title	Compound list table print-out is illegible for some settings
Description	1) Load a data file (ie - serotransferrin.d) with mass match results for about 75 compounds. (Limit to 75 compounds in the Find by MFE editor). 2) Configure the Compound List table to have 8-10 columns. 3) Right click in the Compound list pane and select Print command. 4) Select All rows in the Print dialog. 5) In the Options tab of the dialog select "Fit to one page" and landscape orientation. Click OK. The printed spectra is confined to a narrow space on the left hand side of the page and is illegible. Much of the page will be empty. Two pages may be printed instead of one.

Issue # 193630	
Title	Function: changed value messages are missing in Method Editor > Find Compound by Formula - Options > Results tab
Description	1) Select Find compounds by Formula > Find Compounds by Formula -Options in method explorer 2) Open Results tab. 3) Enable Extract raw spectrum option 4) Enable Clip extracted raw spectra option 5) Select Asymmetric (m/z) from dropdown 6) Enter valid values for both input box (such as 6 and 11) Changed value blue triangles with a message should be displayed. Currently, nothing appears there.

Issue # 193718

Title	No blue triangles are added to the method editor for search accurate mass library when switching search accurate mass library to search unit mass library
Description	Adding a library to the Library selection list in the Search Unit Mass Library > Library Search section will also add a blue triangleto the Search Accurate Mass library line in the Method Explorer. This has no impact on usability.

Issue # 193755	
Title	Find by Integration -> Adjust Delay Time tab contains misaligned fields
Description	The headings under: 'Method Editor -> Find by Integration -> Adjust Delay Time' are slightly misaligned. Will not affect usability or legibility

Issue # 194031	
Title	Localization Issue: Error message contains both English and Japanese strings
Description	Trying to print an acquisition report with data without a method file will gnerate an error that contains English and Japanese strings.

Issue # 194053	
Title	Displaying overlaid MRMs then switching from minutes to scans may cause an error
Description	Loading a few MRM files, overlaying them, and then switching from minutes to scans may intermittenly throw an exception. This error is non-fatal and the user may still proceed.

Issue # 194449	
Title	All Ions MS/MS (AIM) - Visualization in the Compound Fragment Spectrum Results window in Compound Details View (CDV) is incorrect
Description	a) The default zoom range in the x-axis is currently not limited, for target compounds, to the mass of the highest selected adduct species multiplied by the charge state plus 20. b) The red isotopic pattern boxes are incorrectly drawn with a factor of 20 too high.

Issue # 194537	
Title	Cell borders are missing in Bioconfirm Protein Compound reports
Description	When printing data files with protein deconvolution results to the compound report template, BioConfirmProteinCompoundReport.xltx, all columns after MaxZ are missing the cell borders.

Issue # 194539	
Title	Oligonucleotide reports will contain some cosmetic discrepancies
Description	1) Select BioConfirmOligonucleotideCompoundReport.xltx in Common Reporting Options.

	2) Load any data file with oligonucleotide results. 3) File -> Print a compound report. 1. The cell borders are missing for all columns after Vol column. 2. The x-axes of EICs and ECCs have overlapping text. This is cosmetic and has no impact on usability or stability.

Issue # 194702	
Title	Localization: "Acquisition Time" axis label in the Chromatogram Result plot is not translated into Japanese
Description	Loading a data file processed in English into the Japanese version of Qual will not have "Acquistion Time" in the x-axis of a Chromatogram Results plot translated into Japanese properly. This is cosmetic and has no impact on usability or stability.

Issue # 194817	
Title	Scrolling anomaly exists in Digest Comparative Analysis window
Description	1) Open two digest data files (for example enolase digest). 2) Select Wizards | Compare Digest Files : Find results... 3) Iimport the corresponding sequence file in the Define Match Sequences page. 4) Complete the rest of the wizard and generate results. In the Comparative analysis window that gets displayed, scroll down Compound Compare List and highlight a row. The scroll position square jumps up to the top and does not stay at the selected position.

Issue # 194818	
Title	Multiple rows cannot be highlighted in Compound Compare List table
Description	1) Open two digest data files (for example enolase digest). 2) Select Wizards | Compare Digest Files : Find results... 3) Iimport the corresponding sequence file in the Define Match Sequences page. 4) Complete the rest of the wizard and generate results. In the Comparative analysis window that gets displayed, highlight a row in Compound Compare List and use the shift key to highlight multiple rows. The user is then unable to highlight the multiple rows.

Issue # 194819	
Title	Chromatogram selection in Digest Compare Results does not work correctly
Description	1) Open two digest data files (for example enolase digest). 2) Select Wizards | Compare Digest Files : Find results... 3) Importi the corresponding sequence file in the Define Match Sequences page. 4) Complete the rest of the wizard and generate results. 5) In the Comparative analysis window do the following actions:

	-With Extracted Compound Chromatogram (ECC's) displayed click inside the Chromatogram Compare Results pane in Comparative Analysis results. -Select Total Ion or Total Compound Chromatogram. -Reselecting Extraction compound or Extracted ion chromatogram will not display the selected chromatogram. It will still display either: Total Ion or Total Compound Chromatogram.

Issue # 194820	
Title	Chromatogram Compare report generation does not work properly
Description	1) Open two digest data files (for example enolase digest). 2) Select Wizards | Compare Digest Files : Find results... 3) Import the corresponding sequence file in the Define Match Sequences page. 4) Complete the rest of the wizard and generate results. 5) In the Comparative analysis window that gets displayed, perform the following actions: -Click on any row in the Compare List table. -Click on the Print icon in Chromatogram Compare Results pane. -Select "All chromatograms" radio button in the Print dialog and click OK. -Two different rows are printed even though only one row was selected. -Select another row and repeat the process. -The selected row is printed in addition to the previously selected rows. This acts as if CTRL key was used in the table.

Issue # 194821	
Title	Mass Spectrum Compare Results printing has several issues
Description	1) Open two digest data files (for example enolase digest). 2) Select Wizards | Compare Digest Files : Find results... 3) Import the corresponding sequence file in the Define Match Sequences page. 4) Complete the rest of the wizard and generate results. In the Comparative analysis window that gets displayed perform the following actions: 5) Click on any row in the Compare List table. 6) Click on the Print icon in Mass Spectrum Compare Results pane. 7) Select "All spectra" radio button in the Print dialog and click OK. Two different rows are printed even though only one row is selected. Select another row and repeat the process. The selected row is printed in addition to the previously selected rows. This acts as if CTRL key was used in the table. -Additionally, when the mass spectrum is the chosen in the combo box of the pane, MFE manufactured spectra are not included. Product ion spectra are included instead, which should not be part of this pane. -Finally, Header and footer information are not given.

Issue # 194822

Title	MSMS Spectrum Compare Results pane has multiple print issues
Description	1) Open two digest data files (for example enolase digest). 2) Select Wizards | Compare Digest Files : Find results... 3) Import the corresponding sequence file in the Define Match Sequences page. 4) Complete the rest of the wizard and generate results. In the Comparative analysis window that gets displayed perform the following actions: 5) Click on any row in the Compare List table. 6) Click on the Print icon in MSMS Spectrum Compare Results pane. 7) Select the "All spectra" radio button in the Print dialog and click OK. Two different rows are printed even though only one row is selected. Select another row and repeat the process. The selected row is printed in addition to the previously selected rows. This acts as if CTRL key was used in the table. -Additionally, "Scan Spectra MFE" manufactured spectra are included, which should not be part of this pane. -Finally, Header and footer information are not given..

Issue # 195162	
Title	F1 doesn't show help in Isotope Distribution Calculator
Description	Pressing F1 in the Isotope Distribution Calculator will not display the help screen. The user will need to manually mouse to the "Help" menu option.

Issue # 195492	
Title	In CDV with BioConfirm ProteinDigest results - scrolling to the end of the Compound List then back up to last seq. match will cause the cursor to slowly self scroll back to end of list/last compound
Description	1) Opn Datafile: enolase-Chip-final.D 2) Load EnolaseMSMS.m if available; if not use BCProteinDigest default method 3) Run MFE - TheEnolase method contains the Enolase sequence If not available load BSADigest.psq or any available sequence file 4) Run Match Sequence. 5) Switch to CDV (Compound Details View) 6) View->Sequence Coverage Map 7) Proceed to Compound ID Results pane 8) Select another row in Compound List The Win7 busy icon (turquoise circle) will appear and the cursor will constantly move from row to row endlessly.

Issue # 195643	
Title	Layouts in Compound Details View (CDV) and Navigator View (NV) do not save and preserve which PANE is on top if multiple windows are TABBED

Description	1) In Navigator View, have the Compound List and the Peak List tabbed at the top, with the Compound List in front. 2) Save the layout, switch to CDV and back to NV The Peak List is now in front. After running the MFE algorithm, there are no results in the peak list. 1) In Compound Details View, display the "Overall Chromatogram Results" window tabbed behind the "Compound Chromatogram Results" window. 2) Switch back and forth between CDV and NV will cause the "Overall Chromatogram Results window to come to the front.

Issue # 195649	
Title	Changing workflows does not work if "Save current method" is checked in the dialog box
Description	Normally, when changing workflows, a dialog comes up. If "Save current method" is checked in that dialog box, no layout change happens.

Issue # 195773	
Title	EIC Peak List table does not get updated in tandem with compound selection
Description	1) Enter 10-20k for the mass range In the Find by Protein Deconvolution method editor. 2) Select TIC and Extract EIC in the results tab. 3) Run Find by Protein Deconvolution for BetaLac.d. 4) Highlight the compounds in the compound list table one at a time. -The MS Peaks Two table does not always gets updated to correspond to the highlighted compound. This will not impact usability or stability.

Issue # 195933	
Title	If only "Other (CE)" is marked in the User Interface Configuration dialog box, menu items and method editor sections are not chosen consistently
Description	Mark ONLY "Other (CE)" in the User Interface Configuration dialog box for the separation type. 1) “Find by Targeted MS/MS” algorithm is available in the Method Explorer, but is not listed in the “Find” menu. 2) In the Method Explorer, the only “Identify Compounds” section that is available is “Combine Identification Results”. However, in the “Compound Automation Steps” section, all of the Compound identification algorithms can be marked. 3) Database Search tabs and the Generate Formulas tabs in the Chromatogram Peak Survey Workflow are also accessible. (but not in the Identify section of the method editor) 4) In the "Identify" menu, the menu item “Search Library for Spectra” is available, but the selected library cannot be changed because those sections are not available in the "Identify" section of the Method Editor.

Issue # 196295	
Title	Exception occurs in Metlin - Navigator View while repeatedly printing reports over and over for thousands of compounds per data file
Description	The following exception will flag in this case: Program: Agilent MassHunter Workstation Software Qualitative Analysis B.06.00 Build Configuration: Release Message: Following exception occured while exceuting script - Error creating window handle. At- at System.Windows.Forms.NativeWindow.CreateHandle(CreateParams cp) at System.Windows.Forms.Control.CreateHandle() at System.Windows.Forms.Control.get_Handle() at System.Windows.Forms.Control.CreateGraphicsInternal() at System.Windows.Forms.Control.CreateGraphics() at Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.WritePlotImageToFile(IAppState appState, ExportedImageType imageType, UIUpdateDisplayPlotControlBase plotControl, Double heightByWidthRatio, String imageFilename) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.CreatePlotImageFile(IDataItem plotItem, ExportedImageType imageType, Boolean overlayPredictionPattern, IRange XZoomRange, Double heightByWidthRatio, Boolean allowZoom) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.WritePlotPairs(IDataItem[] plots, Int32 ItemID) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CompoundReportGenerator.WriteCompoundChromatograms(IDataItem plotItem, List`1 cpdChildren, Boolean& hasAllIonsResults) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CompoundReportGenerator.WriteCompounds(IDataItem[] compounds) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CompoundReportGenerator.GenerateReportSpecialized(IDataItem[] selectedAnalysis) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.GenerateReportAndMapExceptions(IDataItem[] analyses) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.GenerateReport(IDataItem[] selectedAnalysis) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CmdGenerateReport.DoSpecialized() at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualCommandBase.Do() at Agilent.MassSpectrometry.CommandModel.CommandHistory.Invoke(ICommand cmd) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.AppManager.Invoke(ICommand cmd) Stack Trace: Server stack trace: at Agilent.MassSpectrometry.DataAnalysis.Qualitative.AppManager.BeginRun(String

	assemblyPath, QualScriptEnvironment qualScriptEnvironment) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualCommandBase.RunScript(String script, QualScriptParameters scriptParams, ActionItemCollection actions) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualCommandBase.RunScripts(String[] scripts, QualScriptParameters scriptParams, ActionItemCollection actions) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CmdRunScript.DoSpecialized() at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CmdApply.DoSpecialized() at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualCommandBase.Do() at Agilent.MassSpectrometry.CommandModel.CommandHistory.Invoke(ICommand cmd) at System.Runtime.Remoting.Messaging.StackBuilderSink._PrivateProcessMessage(IntPtr md, Object[] args, Object server, Int32 methodPtr, Boolean fExecuteInContext, Object[]& outArgs) at System.Runtime.Remoting.Messaging.StackBuilderSink.PrivateProcessMessage(RuntimeMethodHandle md, Object[] args, Object server, Int32 methodPtr, Boolean fExecuteInContext, Object[]& outArgs) at System.Runtime.Remoting.Messaging.StackBuilderSink.AsyncProcessMessage(IMessage msg, IMessageSink replySink) Exception rethrown at [0]: at System.Runtime.Remoting.Proxies.RealProxy.EndInvokeHelper(Message reqMsg, Boolean bProxyCase) at System.Runtime.Remoting.Proxies.RemotingProxy.Invoke(Object NotUsed, MessageData& msgData) at Agilent.MassSpectrometry.CommandModel.CommandHistory.InvokeCommand.EndInvoke(IAsyncResult result) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.AppManager.EndInvoke(IAsyncResult result) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualForm.OnAsyncCallBack(IAsyncResult asyncResult) Message: Error creating window handle. Stack Trace: at System.Windows.Forms.NativeWindow.CreateHandle(CreateParams cp) at System.Windows.Forms.Control.CreateHandle() at System.Windows.Forms.Control.get_Handle() at System.Windows.Forms.Control.CreateGraphicsInternal() at System.Windows.Forms.Control.CreateGraphics() at Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.WritePlotImageToFile(IAppState appState, ExportedImageType imageType, UIUpdateDisplayPlotControlBase plotControl, Double heightByWidthRatio, String imageFilename) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.CreatePlotImageFile(IDataItem plotItem, ExportedImageType imageType, Boolean overlayPredictionPattern, IRange XZoomRange, Double heightByWidthRatio, Boolean allowZoom) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.WritePlotPairs(IDataItem[] plots, Int32 ItemID) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CompoundReportGenerator.WriteCompoundChromatograms(IDataItem plotItem, List`1 cpdChildren, Boolean& hasAllIonsResults)

	at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CompoundReportGenerator.WriteCompounds (IDataItem[] compounds) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CompoundReportGenerator.GenerateReportSpecialized(IDataItem[] selectedAnalysis) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.GenerateReportAndMapExceptions(IDataItem[] analyses) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.BaseReportGenerator.GenerateReport(IDataItem[] selectedAnalysis) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.CmdGenerateReport.DoSpecialized() at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualCommandBase.Do() at Agilent.MassSpectrometry.CommandModel.CommandHistory.Invoke(ICommand cmd) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.AppManager.Invoke(ICommand cmd)

Issue # 196296	
Title	Exception on generating Compound Report for ForensicsTox Find by Formula analysis
Description	When running reports on 1000's of compounds per multiple files, Excel stops and opens the Visual Basic debugger at a formatting statement.

Issue # 196507	
Title	Color coding of ions based on Fragment Anotation is still displayed when Fragment Anotation is unchecked
Description	Unchecking "Annotate Fragment Specturm Peaks with Formula" in "Method Editor: Generate Formula -> Fragment Formula" will cause the formulas to disappear but leave the ions that match the formulas colored.

Issue # 196599	
Title	All Ions: ?? appearing on "delete" and "extract complete result set".
Description	1) Run All Ions FbF 2) Select a compound 3) Delete All fragment ion EIC objects (Right click delete on treeview) 4) Extract complete result set 5) Delete All fragment ion EICs objects (Right click delete on treeview) 6) Extract complete result set. 7) ?? will appear in the description

Issue # 196720	
Title	MS/MS Formula details disappear when selecting a different "Best" Formula after running Find Compounds by Auto MS/MS and MFG
Description	1) Run Find Compounds by Auto MS/MS on "Sulfa-PosESIAutoMSMS-c.d", 2) Run Generate Formula from Compounds. 3) Select Compound 10 with m/z 311.0814 and look at MS/MS Formula Details window, which shows the fragment ion results. 4) Select a different "Best" formula, and the MS/MS Formula Details window will

	display "No Formula Results for this compound". Even changing the selection of "Best" back to the correct formula with the highest score will leave this window empty. **Temporary Solution:** The only way to recover the results in MS/MS Formula details is to rerun "Generate Formulas from Compounds"..

Issue # 196721	
Title	The "Hide Empty Columns" tool button in the Compound List works for the first level, but not the second level
Description	The "Hide Empty Columns" tool button in the Compound List works for the first level, but not the second level. This will not impact usability or stability.

Issue # 196722	
Title	Compound List column order for BioConfirm Protein Digest is randomly ordered.
Description	Opening any protein digest file will display compound list columns that are randomly ordered.

Issue # 196831	
Title	In Compound Details View, right-clicking near an axis in the Compound Chromatogram window will throw an error.
Description	1. Generate compounds by performing FbF or MFE. 2. Switch to Compound Details View (CDV) 3. Right click on the gray area (of the x or y-axes, not on the plot directly) on the Compound Chromatogram Results window The following error is thrown: Program: Agilent MassHunter Workstation Software Qualitative Analysis B.06.00 Build Configuration: Debug Message: Object reference not set to an instance of an object. Stack Trace: at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualCpdChromPlotControl.ChromPlotMenu_Opened(UIDisplayPlotContextMenuEventArgs ePlot) in z:\Archer\QualCommon\QualCommonUI\QualCommonUI\pspl_sources\QualCpdChromPlotControl\QualCpdChromPlotControl_3.cs:line 764 at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualCpdChromPlotControl.UIComponent_ShowContextMenu(Object sender, UIDisplayContextMenuEventArgs e) in z:\Archer\QualCommon\QualCommonUI\QualCommonUI\pspl_sources\QualCpdChromPlotControl\QualCpdChromPlotControl_3.cs:line 921.

Issue # 196842

Title	Merged Spectrum ID Results with LibSearch-MFG results - only the highest Lib Score hit has MFG results and Isotope pattern although all are labeled as merged LibSearch-MFG.
Description	1) Select ranges for the three largets peaks in the TIC 2) Integrate & Extract Spectra -> Over Selected Ranges 3) Highlight spectrum. 4) Search unit mass library NIST11.L or Wiley9th.L for spectra from right-click menu in MS Spectrum Results 5) Run "Generate Formula from Spectrum Peaks" 6) Expand "Best merged hit - MFG results" Change "best" hit to another merged hit and expand it. There will be no MFG results. The MS Spectrum Results now do not include the Isotope Pattern

Issue # 196930	
Title	Spectrum not seen on printed report when grid lines are turned on.
Description	If grid lines are turned on, printing an analysis report for all compounds will not display the spectrum chromatograms in the User Spectra section. Only the mass labels will be visible. **Temporary Solution:** Turn off grid lines via plot options and then print.

Issue # 196936	
Title	A Compound report after running MFE + MFG contains 3 columns with the identical formula.
Description	1) Run MFE and then "Generate formulas from compounds" 2) Print the default compound report and the compound list contains three columns with the titles "Formula", "MFG Formula" and "DB Formula", which will all list the same formula (best hit for each compound). **Temporary Solution:** Create a specific report layout for MFE+MFG and only include the appropriate column.

Issue # 196939	
Title	When run as a Compound Automation Step, Find Compounds by MRM produces a TIC Scan with NO DATA POINTS.
Description	This occurs on any MRM or DMRM data file when Find Compounds by MRM is run via Compound Automation. **Temporary Solution:** Run Find Compounds by MRM manually.

Issue # 197052	
Title	Qual crashes when Find by Protein Deconvolution is attempted under specific conditions

Description	1) Open BioConfirmIntactProtein-default.m method. 2) OpenBetaLac and BGALA data sets. 3) In Find by Protein Deconvolution method editor, select "Pmod" as the algorithm. 4) Enter 10000-150000 in Mass Range field 5) Select Extract EIC and BPC in the Results tab 6) Select "Universal" as integrator in the Find by Protein Deconvolution method editor. 7) Select Actions -> Find by Protein Deconvolution. This causes Qual to crash..

Issue # 197054	
Title	Protein compound report with two data sets may fail
Description	1) Open BioConfirmIntactProtein-default.m method. 2) Open BetaLac and BGALA data sets. 3) In Find by Protein Deconvolution method editor Enter 10000-150000 in Mass Range field 4) Select "Use limited m/z range" and "Unspecified" for Isotope width. 5) Select Extract EIC in the Results tab. 6) Select Actions -> Find by Protein Deconvolution. 7) Select File -> Print -> Compound Report. 8) Select All results, and Separate report per data file, 9) Print preview in the Print Comp Rep dialog and click OK. Only one report gets produced and after that it generates error. NOTE: This MAY happen sporadically.

Issue # 197064	
Title	Compound Details View (CDV) - Exception when trying to access the Add/Remove Columns dialog in the 4th level of the Compound ID Results Window
Description	In the Compound Details View (CDV), after running MFE + Sequence Match for BioConfirm, and then trying to access the Add/Remove Columns dialog in the 4th level of the Compound ID Results Window, the user is getting the following exception: Build Configuration: Release Message: Object reference not set to an instance of an object. Stack Trace: at Agilent.MassSpectrometry.DataAnalysis.Qualitative.SelectCompoundColumnDialog..ctor(IResultAttributeDefinitions definition) at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualForm.AddRemoveColumnsMenuItems_Click(Object sender, ToolClickEventArgs e) in t:\Archer\qual\presentation\AgtQual\QualFormP5ViewMenus.cs:line 5176 at Agilent.MassSpectrometry.DataAnalysis.Qualitative.QualForm.UltraToolbarsManager1_ToolClick(Object sender, ToolClickEventArgs e) in t:\Archer\qual\presentation\AgtQual\QualFormP6MenuStates.cs:line 2128 Clicking OK on this error message will NOT crash Qual.

Issue # 197212	
Title	Tooltip of Method Explorer is not properly updated
Description	1) Launch Qual 2) Hover over the Method Explorer pane: it should display the last name of the last method loaded. 3) Open new method and check the tooltip of Method Explorer. The tooltip still displays the previous method's name. This has no impact on usability.

Issue # 197263	
Title	Annotation does not work properly for a HighE spectrum
Description	In the MS Spectrum Results window, annotation does not work properly if the spectrum is a HighE spectrum. 1) Find compounds by formula an an All Ions data file. 2) Add an annotation to the peak at 920 for compound 3 (Crimidine) in the HighE Scan. - Cannot zoom into the baseline. - Can add an annotation, but cannot double-click on the annotation to show the annotation dialog box. - Right-click the annotation; can click the Annotation Properties menu item, but the annotation dialog box is not opened. - The toolbar buttons are all greyed out. - The menu items to "Select All Annotations", "Delete Selected Annotations", and "Delete All Annotations" are all greyed out.

Issue # 197273	
Title	Formula and Mass Calculators do not contain GC/Q-TOF parameters when a GC/Q-TOF method is loaded
Description	When a GC/Q-TOF method is loaded, both the mass and formula calculator tools have the "H" selected instead of an electron. Additionally, the formula calculator has "even electron" selected in "MS ion electron state" instead of "allow both even and odd."

Issue # 197404	
Title	Chemical Data Dictionary Editor tabs do not display the relevant help topics
Description	Opening: Sequence -> Chemical Data Dictionary Editor and then pressing F1 will not display that specific tab's relevant help topic. Instead, the help topic displayed is for the Chemical Data Dictionary Editor dialog box.

Issue # 197514	
Title	Wizard pages do not display relevant help topics
Description	All options in the Wizard menu item do not properly display their relevant help topics

	when the F1 key is pressed.

Issue #	
Title	
Description	

Appendix A. Glossary

Term / Acronym	**Definition**
UI	User Interface. The visual representation of the software with which a user interacts.